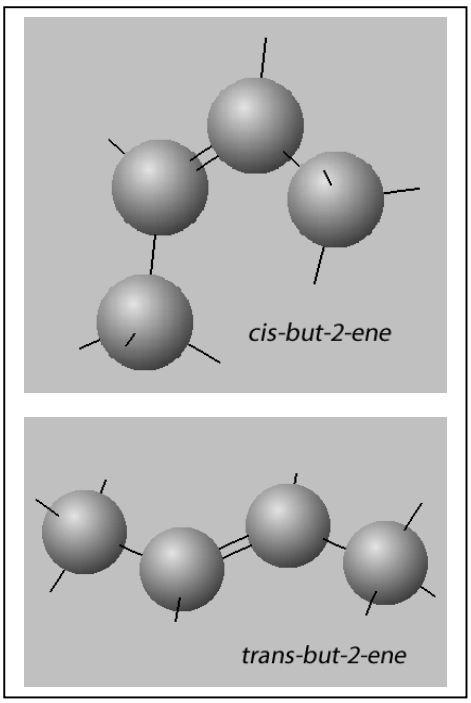
Friday worksheet 10

Organic – trends, chirality, isomers, atom economy and percentage yield.

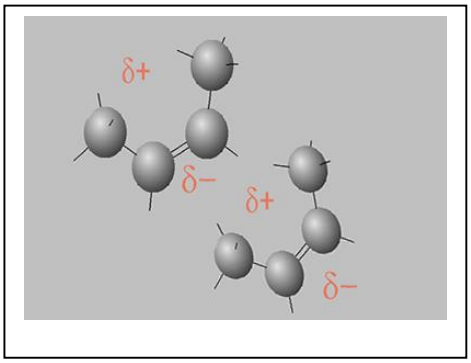
1) Consider the table on the right. Account for the difference in the given physical properties of the cis and trans isomers of butane.

isomer	melting point (°C)	boiling point (°C)
cis-but-2-ene	-139	4
trans-but-2-ene	-106	1

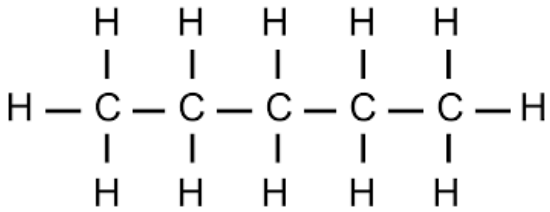
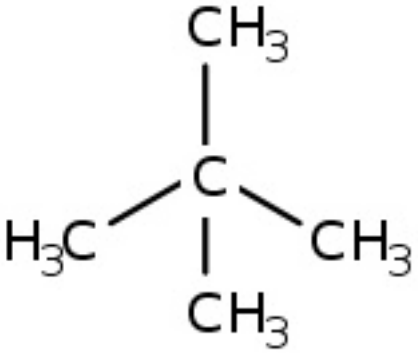
The intermolecular forces of both cis and tans but-2-ene are solely dispersion forces. These forces act over small distances and as such molecules must pack tightly together to allow the relatively weak dispersion forces to exert a force of attraction. In the solid crystal structure the kinked cis isomer cannot pack as tightly as the more linear trans isomer. This causes weaker forces of attraction to exist between molecules in the solid state of the cis isomer as compared to the trans isomer where molecules can pack tighter and hence dispersion forces exert a stronger force of attraction.

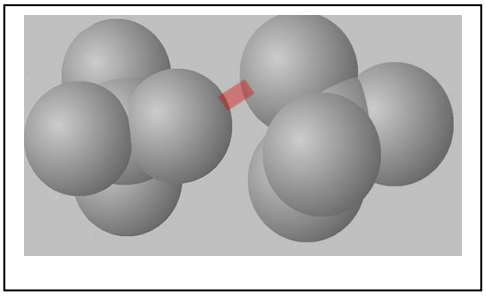


Cis isomers have dipoles across the double bond, as shown on the right, while the trans isomer has no such dipoles across the double bond. In the liquid state where molecules are free to move about these dipoles can move to positions where they can exert a force of attraction. In the liquid state, therefore, cis isomers have dipole-dipole as well as dispersion forces acting between the molecules as compared to the trans isomers that have only dispersion forces. This causes a greater boiling temperature to exist for the cis isomer as compared to the trans isomer.



2) Consider the table below.

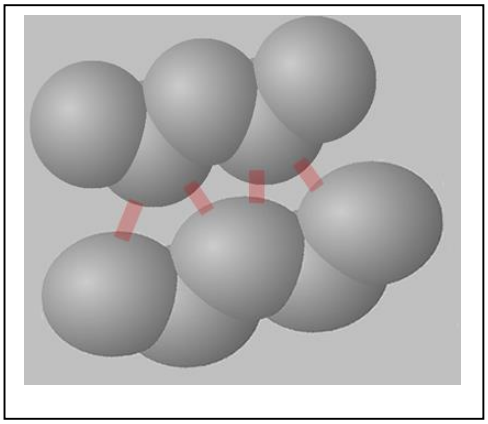
Molecule	Structural formula	Type of intermolecular bonding	Boiling point °C
Pentane		Dispersion forces only	36
2,2-dimethylpropane		Dispersion forces only	10



a. Complete the table.

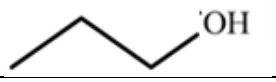
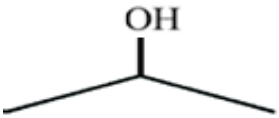
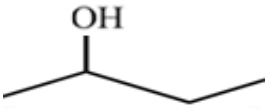
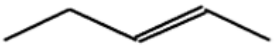
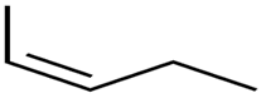
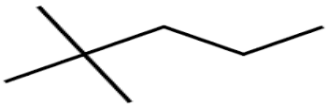
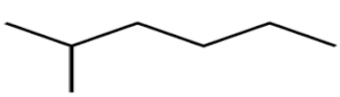
b. Account for the difference in boiling temperature of the two molecules, with identical chemical formula (C_5H_{12}).

Since 2,2-dimethylpropane is a spherical (tetrahedral) shaped molecule, it has less surface area exposed to the other molecules through which it can form weak bonds. Pentane, on the other hand is a linear molecule and has a greater surface area through which it can form intermolecular bonds. This is shown in the image on the right.



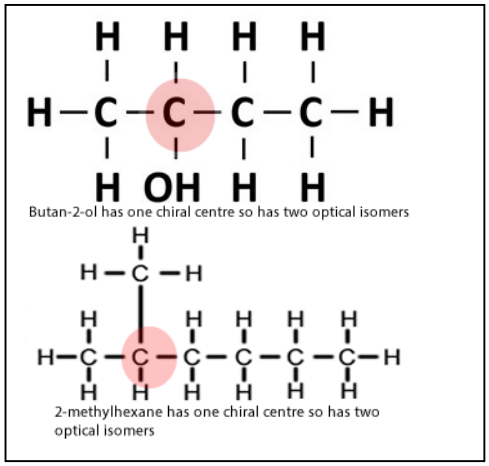
3) Consider the table below.

a. Complete the table.

Name of molecule	Skeletal formula	Condensed formula
Propan-1-ol		*$CH_3CH_2CH_2OH$*
Propan-2-ol		*$CH_3CH(OH)CH_3$*
Butan-1-ol		*$CH_3(CH_2)_2CH_2OH$*
Butan-2-ol		*$CH_3CH(OH)CH_2CH_3$*
trans-pent-2-ene		*$CH_3CHCHCH_2CH_3$*
cis-pent-2-ene		*$CH_3CHCHCH_2CH_3$*
2,2-dimethylpentane		*$CH_3C(CH_2)_2(CH_2)CH_3$*
2-methylhexane		*$CH_3CH(CH_2)(CH_2)_3CH_3$*

b. i. State the molecules that have isomers that can rotate plane-polarised light in different directions and give the number of isomers that each molecule has.

Molecules with optical isomers have at least one chiral centre. Butan-2-ol , 2-methylhexane



ii. What type of isomers do these two compounds represent?
Optical isomers
iii. Which two molecules represent structural isomers?
2,2-dimethylpentane, 2-methylhexane
iv. Which two molecules are isomers that have similar chemical properties but different physical properties? *cis-pent-2-ene and trans-pent-2-ene*

v. Name the group that the isomers in iv. above belong to. *Geometric isomers*

vi. In the space provided on the right draw the skeletal formula and name another structural isomer of these two compounds that has the highest melting point of the three. Explain why.

Heptane

Heptane is a linear molecule that can pack closely in the solid crystalline structure. Since the intermolecular bonding of all three isomers , *2,2-dimethylpentane, 2-methylhexane and heptane are dispersion forces only, then distance between molecules is critical. Isomers such as 2,2-dimethylpentane and 2-methylhexane are branched and as such cannot pack close together where dispersion forces can exert a greater force of attraction.*

4) Hydrogen is produced using methane gas via two methods as shown below.

i. $CH_4 + H_2O\ (+ \text{heat}) \rightarrow CO + 3H_2$

ii. $2CH_4 + O_2 \rightarrow 2CO + 4H_2\ (+ \text{heat})$

a. Which is the most efficient way which creates the least amount of waste?

Calculate the atom economy of each reaction
i. mass of reactants = (12 + 4) + (16 + 2) = 34
mass of desired product (3 X 2) = 6
=> (6/34) X 100 = 17.6%

ii. mass of reactants = 2 X (12 + 4) + (16 X 2) = 64
mass of desired product (8 X 2) = 16
=> (16/64) X 100 = 25.0%

Reaction ii. has the highest atom economy.

b. 300.23 litres of methane gas at 25.0 °C and 101.3 kPa pressure was reacted with excess steam to produce carbon monoxide and 50.01 grams of hydrogen gas.

i. What is the percentage yield for the reaction to the right number of significant figures?

Percentage yield = (actual mass of product) / (theoretical mass of product) X 100

⇨ *Theoretical mass of hydrogen*
=> $mol_{methane}$ = PV/RT = (101.3 X 300.23) / (8.31 X 298) = 12.28 mol
=> $mol_{hydrogen}$ = 12.28 X 3 = 36.84 mol
=> mass $_{hydrogen}$ = 36.84 X 2.00 = 73.7 grams
Percentage yield
=> actual/ theoretical X 100 = (50.01 / 73.7) X 100 = 67.9%

ii. Using Le Chatelier's principle discuss two ways to increase the yield in a timely manner to meet the demand of an industrial production process.

Any two of the following
- Perform the reaction at high temperatures
- Use excess steam with a suitable catalyst.
- Constantly remove CO from the mixture.
- Decrease the pressure of the reaction vessel in the presence of a suitable catalyst.

iii. Hydrogen gas produced by either of the two reactions is not considered a green and renewable fuel. Explain why and describe under what conditions may hydrogen be considered a green and renewable fuel?
Hydrogen derived from methane can be considered a renewable and green fuel depending on where the methane was sourced from. If methane was sourced from the petrochemical industry then the hydrogen is not renewable nor green. If the methane was sourced from the decay of organic matter (biomass), as occurs in rubbish tips, then the hydrogen is renewable and green.